Tutorial 1: Numerical differentiation and integration

Problem 1: Numerical differentiation

Discrete derivatives do not necessarily have to be evaluated at the data points in a given data set. They can also be evaluated halfway between data points to obtain more accuracy.

Derive the discrete formula for the first derivative at $x_{i+1/2}$ using the points at $i$ and $i+1$ on an equispaced grid with $x_{i+1} - x_i = \Delta x$.

Answer

1. The Taylor series expansions about $x_{i+1/2}$ to obtain $f_i$ and $f_{i+1}$ are given by

$$f_{i+1} = f_i + \frac{\Delta x}{2} f'_{i+1/2} + \frac{1}{8} \Delta x^2 f''_{i+1/2} + O(\Delta x^3),$$

$$f_i = f_{i+1} - \frac{\Delta x}{2} f'_{i+1/2} + \frac{1}{8} \Delta x^2 f''_{i+1/2} + O(\Delta x^3).$$

Subtracting the second from the first yields

$$f_{i+1} - f_i = \Delta x f'_{i+1/2} + O(\Delta x^3), \hspace{1cm} (1)$$

which yields the second order accurate compact centered difference approximation of $f'_{i+1/2}$ as

$$f'_{i+1/2} = \frac{f_{i+1} - f_i}{\Delta x} + O(\Delta x^2). \hspace{1cm} (2)$$

Problem 2: Numerical integration

The simplest way to approximate the integral of a function $f(x)$ over the interval $[a,b]$ is to use the rectangular rule, which approximates the function over the interval $[x_i, x_{i+1}]$ as a constant and equal to $f(x_i)$.

1. Write a function, rect, that computes the integral of an arbitrary function $f$ on an equispaced grid $x$ using the rectangular rule, so that in Octave, the function is used as

`>> I = rect(x,f);`

2. Using this function, compute the value of

$$\operatorname{Erf}(1) = \frac{2}{\sqrt{\pi}} \int_0^1 e^{-x^2} \, dx, \hspace{1cm} (3)$$
and show that the rectangular rule is first order accurate with respect to the grid spacing \( h \). Use \( N = 20, 40, 80, 160, 320, \) and \( 640 \) intervals to discretize \( x \) with \( x_i = (i - 1)h, \ i \in \{1, \ldots, N + 1\} \) and \( h = 1/N \), and plot the error as a function \( h \). The error is given by

\[
\text{Error} = \left| \frac{\text{Erf}_N(1) - \text{Erf}_{\text{exact}}(1)}{\text{Erf}_{\text{exact}}(1)} \right|,
\]

where \( \text{Erf}_N(1) \) is the estimate you get using the rectangular rule with \( N \) intervals, and \( \text{Erf}_{\text{exact}}(1) \) is the “exact” value given to you by the erf function in Octave.

**Answer**

Please see the help contents for Octave at:

http://www.octave.org/doc/octave_toc.html

1. The Octave code for the rect function is given below. It can be downloaded from:

   http://fluid.stanford.edu/~fringer/courses/uwc/downloads/rect.m

   ```octave
   %
   % Introduction to numerical methods for finance students
   % Tutorial 1 Problem 2: rect function
   % 09/08/02
   % Oliver Fringer
   %
   % This m-file computes the integral of a function f over the
   % equally spaced points x using the rectangular rule.
   %
   function I = trapz(x,f)

   h = x(2)-x(1);
   N = length(f);
   I = 0;
   for n=1:N-1,
     I = I + h*f(n);
   end

   endfunction
   ```

2. The Octave code to plot convergence is given below. It can be downloaded from:

   http://fluid.stanford.edu/~fringer/courses/uwc/downloads/rect_converge.m
This m-file computes the integral of Erf(1) using the rectangular rule and plots the convergence results.

Integration limits for Erf(1) = 2/sqrt(pi) \int_0^1 e^{-x^2}dx

a = 0;
b = 1;

Cases to compute

Ns = [20 40 80 160 320 640];
Ner = length(Ns);

To store the error values.

ers = zeros(1,Ner);

Compute the integral for each case

for n=1:Ner,

Set up the grid
N = Ns(n);
h = (b-a)/N;
x = [a:h:b];

Gaussian function to be used for the erf integral
f = 2/sqrt(pi)*exp(-x.^2);

The rectangular rule
ers(n) = abs((rect(x,f)-erf(b))/erf(b));
end
% Array containing the grid spacings.
% hs = (b-a)./Ns;

% Loglog plot of the error, showing the hs line
% loglog(hs,ers,"bx;Rectangular;",...
    hs,hs,"x-;h;"
);xlabel('h');ylabel('Error');

The convergence result for the rectangular rule is shown in Figure 1. Convergence is first order accurate because the rectangular rule approximates the function in the range \([x_i, x_{i+1}]\) as

\[
f(x) = f_i + (x - x_i)f_i' + \frac{1}{2}(x - x_i)^2f_i'' + \mathcal{O}\left((x - x_i)^3\right), \tag{5}
\]

So that the integral in a subinterval is given by

\[
\int_{x_i}^{x_{i+1}} f(x) \, dx = \int_{x_i}^{x_{i+1}} f_i \, dx + \frac{1}{2}(x - x_i)^2f_i'' + \mathcal{O}\left((x - x_i)^3\right) \, dx,
\]

\[
= hf_i + \frac{1}{2}h^2f_i' + \mathcal{O}\left(h^3\right), \tag{6}
\]

The integral over the domain \([a, b]\) is then given by

\[
\int_a^b f(x) \, dx = \sum_{i=0}^{N-1} \int_{x_i}^{x_{i+1}} f(x) \, dx,
\]
\[ \begin{align*}
&= h \sum_{i=0}^{N-1} f_i + \frac{1}{2} h^2 N f'(\xi), \\
&= h \sum_{i=0}^{N-1} f_i + \frac{1}{2} h(b - a)f'(\xi), \\
&= h \sum_{i=0}^{N-1} f_i + \mathcal{O}(h),
\end{align*} \]

(7)

where we have used the same arguments to derive the error term as we used in Lecture 5.